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PLANAR HETEROSTRUCTURE
GRAPHENE — NARROW-GAP SEMICONDUCTOR — GRAPHENE

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We investigate a planar heterostructure composed of two graphene films separated by a narrow-gap semiconductor ribbon. We show that there is no the Klein paradox when the Dirac points of the Brillouin zone of graphene are in a band gap of a narrow-gap semiconductor. There is the energy range depending on an angle of incidence, in which the above-barrier damped solution exists. Therefore, this heterostructure is a “filter” transmitting particles in a certain range of angles of incidence upon a potential barrier. We discuss the possibility of application of this heterostructure as a “switch”.

Graphene is a two-dimensional gapless semiconductor, and charge carriers are massless Dirac fermions [1]. It is known [2] that a massless relativistic particle with spin 1/2 possesses the chirality property, i.e. it is characterized by a certain spin projection onto its momentum. In case of graphene, the chirality is defined by a projection of pseudospin onto a momentum direction, which is positive for electrons but negative for holes near K point of the Brillouin zone (BZ) [3], i.e. an electron and a hole are analogues of a massless neutrino with the right- and left-hand helicities, respectively. However, the situation is inverse near K' point where electrons and holes have the left- and right-hand helicities, respectively, [4, 5]. The massless relativistic particle is described by one spinor, i.e. a two-component wave function [6, 7]. It gives basis to state that the effective Hamiltonian describing the charge carriers in graphene near K point is a 2×2 matrix, and corresponding equation is the Weyl equation²

$$u\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}\psi = E\psi, \quad (1)$$

where $u = 9.84 \times 10^7$ cm/s is the Fermi velocity which is an analogue of the Kane matrix element for the rate of interband transitions in the Dirac model [10], $\hat{\mathbf{p}} = -i\hbar\nabla$ (hereafter

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²The massless fermions considered separately near K and K' points are similar to the Weyl (two-component) neutrino. The Dirac equation is used for its simultaneous description [8]. The Dirac equation is equivalent to a pair of the Weyl equations. The Dirac equation in two-dimensions can be written as a 2×2 matrix (it can be used equivalently with a 4×4 matrix representation) which coincides with the Weyl equation for a massless particle on a plane. However, the former equation can be also used for a description of a particle with finite mass. Using this fact, the problem very close to considered in this paper task was earlier solved by Gomes and Peres [9].

$\hbar = 1$), and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the Pauli matrices. The dispersion relation of the charge carriers is linear in momentum k

$$E = \pm uk. \quad (2)$$

A narrow-gap semiconductor is described by the 4×4 matrix Dirac equation [11]

$$\hat{H}_D \Psi = \{\bar{u} \boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta \Delta + V_0\} \Psi = E \Psi, \quad (3)$$

where Ψ is a bispinor, \bar{u} is the Kane matrix element for the rate of interband transitions, $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$ are the Dirac α -matrices, $\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$, I is the 2×2 unit matrix, Δ is half the band gap, and V_0 is the difference of work functions of the narrow-gap semiconductor and graphene ($|V_0| < \Delta$).

It is necessary to introduce the four-component wave function, bispinor, for simultaneous description of the charge carriers in graphene and the narrow-gap semiconductor. In this case, the Dirac Hamiltonian is

$$\hat{H}_D = \begin{pmatrix} 0 & u \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} \\ u \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} & 0 \end{pmatrix}. \quad (4)$$

Hamiltonian (4) is equivalent to Hamiltonian used in Ref. [8], with an accuracy of two consecutively performed unitary transformations $\hat{U}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ I & -I \end{pmatrix}$ and $\hat{U}_1 = \begin{pmatrix} I & 0 \\ 0 & \sigma_y \end{pmatrix}$ [12]. In addition, both left-hand and right-hand helicity massless fermions are presented in the system. Transitions between K and K' points are improbable, so it is possible to consider that particles conserve the chirality property.

By performing the unitary transformation \hat{U}_2 , it is convenient to present the Dirac Hamiltonian describing the charge carriers in the total heterostructure (Fig. 1(a)) in the form in which diagonal blocks contain momentum operators

$$\hat{H}'_D = \begin{pmatrix} u_i \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} + V_i & \Delta_i \\ \Delta_i & -u_i \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} + V_i \end{pmatrix}, \quad (5)$$

where $u_1 = u_3 = u$, $V_1 = V_3 = 0$, and $\Delta_1 = \Delta_3 = 0$ are the parameters related to graphene, $u_2 = \bar{u}$, $V_2 = V_0$, and $\Delta_2 = \Delta$ are the parameters of the narrow-gap semiconductor (Fig. 1(b)).

For the components of the bispinor describing a particle in graphene, the following equalities exist

$$\begin{aligned} \psi_2 &= s \psi_1 e^{i\phi}, \\ \psi_4 &= -s \psi_3 e^{i\phi}, \end{aligned} \quad (6)$$

where $\phi = \arctan \frac{k_y}{k_x}$ is the polar angle of momentum $\mathbf{k} = (k_x, k_y)$ of the charge carriers in graphene (the angle of incidence), $s = \text{sign} E$.

For the components of the bispinor describing a particle in the narrow-gap semiconductor, the following equalities exist

$$\begin{aligned} \psi_3 &= \frac{E - V_0}{\Delta} \psi_1 - \frac{\bar{u} q_x - i \bar{u} k_y}{\Delta} \psi_2, \\ \psi_4 &= -\frac{\bar{u} q_x + i \bar{u} k_y}{\Delta} \psi_1 + \frac{E - V_0}{\Delta} \psi_2, \end{aligned} \quad (7)$$

where

$$\bar{u}^2 q_x^2 = (E - V_0)^2 - \Delta^2 - \bar{u}^2 k_y^2. \quad (8)$$

We find the solution in three ranges: I) $x < 0$, II) $0 < x < D$, III) $x > D$ (D is the width of the narrow-gap semiconductor ribbon, see Fig. 1(a)), taking into account relations (6), (7) and assuming that the solution is oscillating in range II ($q_x^2 > 0$),

$$\Psi_I = \begin{pmatrix} c_1 \\ sc_1 e^{i\phi} \\ c_2 \\ -sc_2 e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + \begin{pmatrix} rc_1 \\ -src_1 e^{-i\phi} \\ rc_2 \\ src_2 e^{-i\phi} \end{pmatrix} e^{i(-k_x x + k_y y)}, \quad (9)$$

$$\Psi_{II} = \begin{pmatrix} a_1 \\ a_2 \\ a_1 \frac{E-V_0}{\Delta} - a_2 \frac{\bar{u}q_x - i\bar{u}k_y}{\Delta} \\ -a_1 \frac{\bar{u}q_x + i\bar{u}k_y}{\Delta} + a_2 \frac{E-V_0}{\Delta} \end{pmatrix} e^{i(q_x x + k_y y)} + \begin{pmatrix} b_1 \\ b_2 \\ b_1 \frac{E-V_0}{\Delta} + b_2 \frac{\bar{u}q_x + i\bar{u}k_y}{\Delta} \\ b_1 \frac{\bar{u}q_x - i\bar{u}k_y}{\Delta} + b_2 \frac{E-V_0}{\Delta} \end{pmatrix} e^{i(-q_x x + k_y y)}, \quad (10)$$

$$\Psi_{III} = \begin{pmatrix} tc_1 \\ stc_1 e^{i\phi} \\ tc_2 \\ -stc_2 e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)}, \quad (11)$$

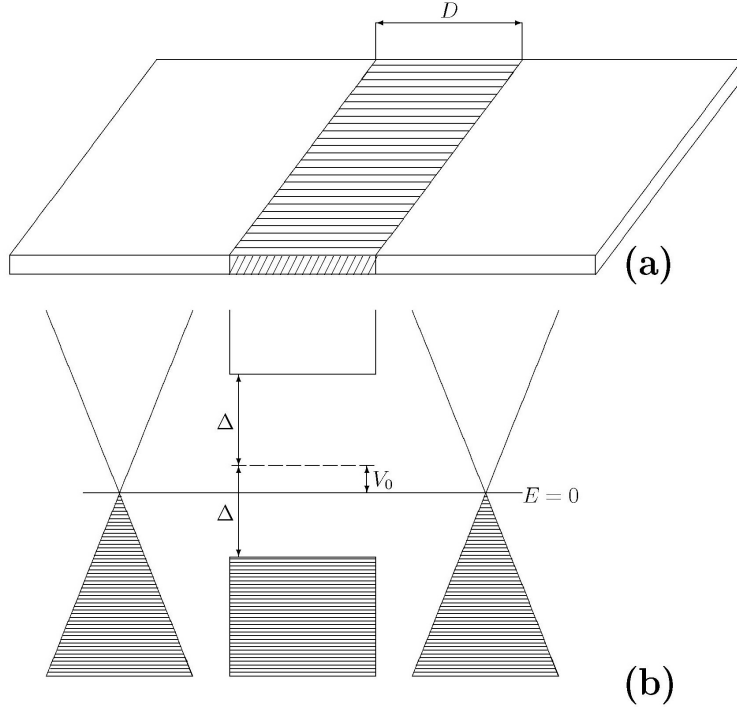


Fig. 1. Considered planar heterostructure; (a) two graphene layers separated by the narrow-gap semiconductor ribbon with the width D (it is hatched), (b) the band structure: level $E = 0$ corresponds to the position of the Dirac points in the BZ of graphene, the band gap of the narrow-gap semiconductor is $E_g = 2\Delta$, V_0 is the difference of the work functions of graphene and the narrow-gap semiconductor, completely filled valence bands are hatched.

where r and t are the reflection and transmission coefficients, respectively, [3], c_1 , c_2 , a_1 , a_2 , b_1 , b_2 are complex constants determined from the boundary conditions³.

Using the boundary conditions [13, 14]

$$\sqrt{u^{(-)}}\Psi^{(-)} = \sqrt{u^{(+)}}\Psi^{(+)}, \quad (12)$$

where the quantities marked by “(−)” and “(+)” relate to material placing on the left and right of the boundary, respectively, we obtain for the transmission coefficient

$$t = \frac{\cos \phi}{\cos \phi \cos(q_x D) + i \left(\tan \theta \sin \phi - s \frac{E-V_0}{\bar{u}q_x} \right) \sin(q_x D)} e^{-ik_x D}, \quad (13)$$

where $\tan \theta = \frac{k_y}{q_x}$. Expression (13) corresponds to the oscillating solution in range II. In order to get the transmission coefficient at the exponentially damped solution in range II, the replacement $q_x \rightarrow i\tilde{q}_x$ should be made where $\bar{u}^2 \tilde{q}_x^2 = \Delta^2 + \bar{u}^2 k_y^2 - (E - V_0)^2$, and $\tilde{q}_x^2 > 0$. The transmission probabilities $T = |t|^2$ for both kinds of solution in range II are

$$T_{\text{oscil}} = \frac{\cos^2 \phi}{\cos^2 \phi \cos^2(q_x D) + \left(\tan \theta \sin \phi - s \frac{E-V_0}{\bar{u}q_x} \right)^2 \sin^2(q_x D)}, \quad (14)$$

$$T_{\text{damp}} = \frac{\cos^2 \phi}{\cos^2 \phi \cosh^2(\tilde{q}_x D) + \left(\frac{k_y}{\tilde{q}_x} \sin \phi - s \frac{E-V_0}{\bar{u}\tilde{q}_x} \right)^2 \sinh^2(\tilde{q}_x D)}. \quad (15)$$

One can see from formula (14) that $T_{\text{oscil}} = 1$ when $q_x D = \pi N$, where N is integer. It corresponds to maxima of the transmission probability shown in Fig. 2 (a)-(d).

As one should expect, the transmission probability in case of the damped solution in range II is exponentially small for sufficiently large width of the narrow-gap semiconductor ribbon $D \gg 1/|\tilde{q}_x|$: $T_{\text{damp}} \sim e^{-2|\tilde{q}_x|D}$. The result of the passage to limit, $\Delta \rightarrow 0$, in (13) coincides with the transmission coefficient t in Ref. [3].

The reflection coefficient is simply obtained

$$r = -i \sin(q_x D) \frac{\cos(\phi - \theta) - s \frac{E-V_0}{\bar{u}k'}}{\cos \phi \cos \theta \cos(q_x D) + i \left(\sin \phi \sin \theta - s \frac{E-V_0}{\bar{u}k'} \right) \sin(q_x D)} \cdot \frac{e^{-i\theta} + s e^{i\phi} \frac{E-V_0+\Delta}{\bar{u}k'}}{e^{-i\theta} - s e^{-i\phi} \frac{E-V_0+\Delta}{\bar{u}k'}}, \quad (16)$$

where $k' = \sqrt{q_x^2 + k_y^2}$. The passage to limit, $\Delta \rightarrow 0$, in (16) is performed by replacements $\frac{E-V_0}{\bar{u}k'} \rightarrow s'$, $\frac{E-V_0+\Delta}{\bar{u}k'} \rightarrow s'$, $s' = \text{sign}(E - V_0)$, the result coincides with formula (4) of Ref. [3].

The reflection probabilities $R = |r|^2$ for both types of solution in range II are

³It should be emphasized that $c_2 = 0$ in the bispinors Ψ_I and Ψ_{III} for the right-hand helicity particle, since, the equality $\frac{1-i\gamma_5}{2}\Psi_R = \Psi_R$, where $\gamma_5 = i\beta$, is valid for the bispinor Ψ_R describing the right-hand helicity particle, and $c_1 = 0$ and the equality $\frac{1+i\gamma_5}{2}\Psi_L = \Psi_L$ is valid in those bispinors for the left-hand helicity particle [2]. Consequently, corresponding components of Ψ_{II} are zero on interfaces (ones are zero everywhere for the damped solution).

$$R_{\text{oscil}} = \frac{[\cos(\phi - \theta) - s \frac{E-V_0}{\bar{u}k'}]^2}{\cos^2 \phi \cos^2 \theta \cot^2(q_x D) + (\sin \phi \sin \theta - s \frac{E-V_0}{\bar{u}k'})^2} \times \frac{1 + 2s \frac{E-V_0+\Delta}{\bar{u}k'} \cos(\phi + \theta) + \frac{(E-V_0+\Delta)^2}{\bar{u}^2 k'^2}}{1 - 2s \frac{E-V_0+\Delta}{\bar{u}k'} \cos(\phi - \theta) + \frac{(E-V_0+\Delta)^2}{\bar{u}^2 k'^2}}, \quad (17)$$

$$R_{\text{damp}} = \frac{\bar{u}^2 \tilde{q}_x^2 \cos^2 \phi + (\bar{u}k_y \sin \phi - s(E - V_0))^2}{\bar{u}^2 \tilde{q}_x^2 \cos^2 \phi \coth^2(\tilde{q}_x D) + (\bar{u}k_y \sin \phi - s(E - V_0))^2}. \quad (18)$$

One can see from (18) that $R_{\text{damp}} \rightarrow 1$ at $|\tilde{q}_x|D \gg 1$. It is simply verified that the following equalities are valid

$$\begin{aligned} T_{\text{oscil}} + R_{\text{oscil}} &= 1, \\ T_{\text{damp}} + R_{\text{damp}} &= 1. \end{aligned} \quad (19)$$

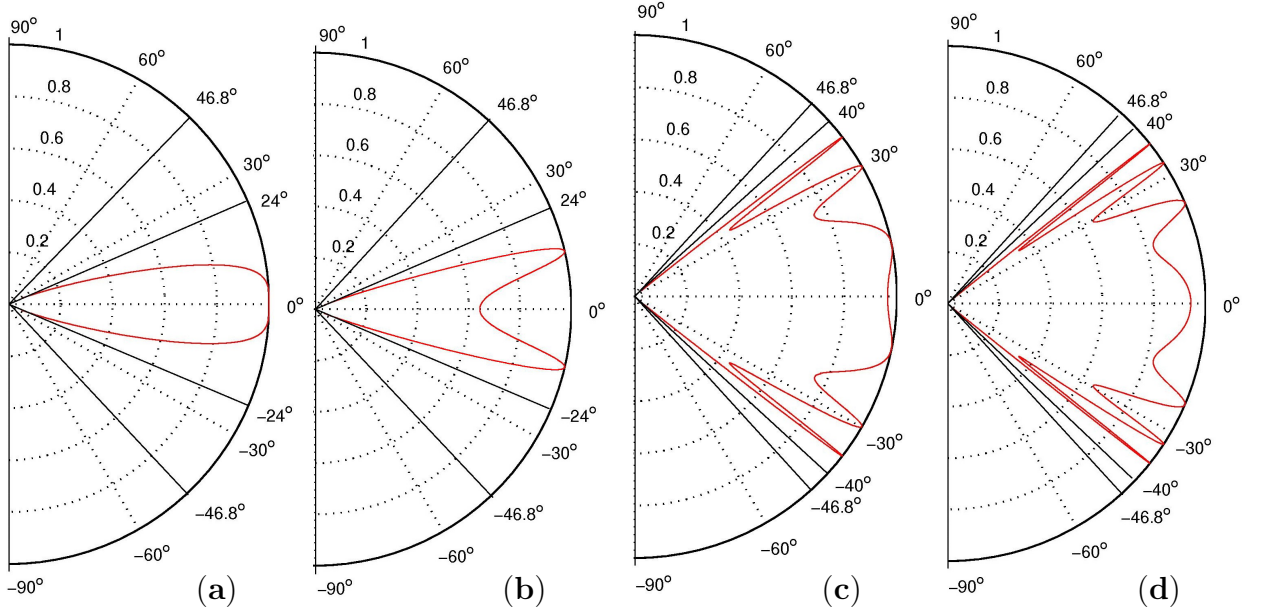


Fig. 2. The dependence of the probability T_{oscil} of the electron transmission through rectangular barrier being the band gap of the narrow-gap semiconductor GaAs with $\Delta = 705$ meV on the angle of incidence, $\bar{u} = \sqrt{\frac{\Delta}{m^*}} = 1.35 \times 10^8$ cm/s where $m^* = 0.068m_0$, m_0 is the free electron mass [16]. The difference of work functions of GaAs and graphene is assumed to be positive and equal in $V_0 = 100$ meV. The angle $\phi_0 \approx 46.8^\circ$ corresponding to the equality $\sin \phi_0 = u/\bar{u}$ is marked. Two values of energy satisfying the above-barrier transmission condition $E > \Delta + V_0$ are considered. When the angle of incidence approaches ϕ_1 , the upper boundary of the above-barrier damped range comes up to the energy E of a incident electron, for $E = 1$ eV $\phi_1 \approx 24^\circ$, for $E = 2$ eV $\phi_1 \approx 40^\circ$: (a) $E = 1$ eV, $D = 50$ Å; (b) $E = 1$ eV, $D = 60$ Å; (c) $E = 2$ eV, $D = 50$ Å; (d) $E = 2$ eV, $D = 60$ Å.

Let us analyze the conditions at which the oscillating or damped solution can exist in range II. For definiteness, we consider the case of electrons⁴: its energy $E = uk$ is positive in graphene, then, for the oscillating solution, the following equality should hold:

$$uk = V_0 + \sqrt{\Delta^2 + \bar{u}^2 q_x^2 + \bar{u}^2 k_y^2}, \quad (20)$$

which is valid at condition

$$uk - V_0 > \sqrt{\Delta^2 + \bar{u}^2 k_y^2}. \quad (21)$$

Conversely, it is necessary for the damped solution⁵ that

$$uk = V_0 + \sqrt{\Delta^2 - \bar{u}^2 \tilde{q}_x^2 + \bar{u}^2 k_y^2}. \quad (22)$$

It is valid at condition of the intersection of the dispersion curves for graphene and the narrow-gap semiconductor [15]

$$uk - V_0 < \sqrt{\Delta^2 + \bar{u}^2 k_y^2}. \quad (23)$$

It is evident from the inequality (23) that if the Dirac point of the BZ of graphene falls into the band gap of the narrow-gap semiconductor (tunneling through the potential barrier being the band gap of the narrow-gap semiconductor) then the solution in range II for electrons with the energy $E_e < V_0 + \Delta$ (analogously for holes with the energy $E_h > V_0 - \Delta$) is always damped one.

The momentum range corresponding to the oscillating solution is defined by inequality

$$(u^2 - \bar{u}^2 \sin^2 \phi) k^2 - 2V_0 uk + V_0^2 - \Delta^2 > 0, \quad (24)$$

and the inverse inequality defines the momentum range of the damped solution. The analysis of inequality (24) shows the following:

1) if $u > \bar{u}$ then at any angle of incidence $-\frac{\pi}{2} < \phi < \frac{\pi}{2}$ for electrons with energy E_e and holes with energy E_h in range

$$\begin{aligned} \Delta + V_0 &< E_e < E^+(\phi), \\ E^-(\phi) &< E_h < -\Delta + V_0, \end{aligned} \quad (25)$$

where $E^\pm(\phi) = \frac{V_0 \pm \sqrt{\Delta^2 - \eta \sin^2 \phi (\Delta^2 - V_0^2)}}{1 - \eta \sin^2 \phi}$, $\eta = \frac{\bar{u}^2}{u^2}$, there is the above-barrier damped solution; in range $E_e > E^+(\phi)$ and $E_h < E^-(\phi)$ there exists the oscillating solution;

2) if $u < \bar{u}$ (it is valid for a number of the narrow-gap semiconductors, e.g., GaAs and InSb) then it is necessary to distinguish the following particular cases:

a) the situation in the range of angles $|\sin \phi| < \frac{u}{\bar{u}}$ is the same as the case 1);

⁴The case of holes is equivalent to the case of electrons with an accuracy of the replacement $E \rightarrow -E$ and $V_0 \rightarrow -V_0$.

⁵The expression with sign minus before the square root can also correspond to the damped solution if $V_0 > 0$ and value of the square root is smaller V_0 .

b) the behavior of particles in the range of angles $\frac{u}{\bar{u}} < |\sin \phi| < 1$ is various depending on the value V_0 :

b*) if $\Delta\sqrt{1 - \frac{u^2}{\bar{u}^2}} < |V_0| < \Delta$ then it should distinguish the subcases for all values of angles from this range:

(i) there is the damped solution at any k (at any energy) for electrons at $V_0 > 0$ and for holes at $V_0 < 0$;

(ii) there is energy range above the barrier for electrons at $V_0 < 0$ and holes at $V_0 > 0$, transparency window, in which there is the oscillating solution, and beyond it there is the damped solution:

$$\begin{aligned} E_1(\phi) &< E_e < E_2(\phi), \\ -E_2(\phi) &< E_h < -E_1(\phi), \end{aligned} \tag{26}$$

where $E_{1,2}(\phi) = \frac{V_0 \mp \sqrt{\Delta^2 - \eta \sin^2 \phi (\Delta^2 - V_0^2)}}{\eta \sin^2 \phi - 1}$;

b**) if $|V_0| < \Delta\sqrt{1 - \frac{u^2}{\bar{u}^2}}$ then

(j) the situation is the same as case b*) in the range of angles $\frac{u}{\bar{u}} < |\sin \phi| < \frac{u}{\bar{u}} \frac{\Delta}{\sqrt{\Delta^2 - V_0^2}}$;

(jj) there exists only the damped solution at any k in range of angles $\frac{u}{\bar{u}} \frac{\Delta}{\sqrt{\Delta^2 - V_0^2}} < |\sin \phi| < 1$.

The potential barrier is an ideal reflector at sufficiently large angles of incidence in cases (i) and (jj), i.e. an “angle filter” transmitting particles with angles of incidence near to $\phi = 0$. At the same time, it is supposed that $|q_x|D \gg 1$, i.e. $T_{\text{damp}} \ll 1$. Such an unusual feature of the rectangular potential barrier is related to the circumstance that the “speed of light”, analogues of which are u and \bar{u} , is different in graphene and the narrow-gap semiconductor [14].

The case $u = \bar{u}$ should be attributed to the case 1). Then the energy range of the above-barrier damped solution disappears, and a particle behaves as an usual nonrelativistic particle, namely, there are the damped and oscillating solutions under and above the barrier, respectively. Similar results in this particular case have been obtained by Gomes and Peres [9].

Let us consider separately the case when we have instead of the narrow-gap semiconductor, a gapless semiconductor for which $\bar{u} \neq u$, and $V_0 \neq 0$ (at $\bar{u} = u$ this case coincides with one considered in [3]). However, in contrast to Ref. [3], there is a number of features distinguished the case $\bar{u} \neq u$. The transmission probabilities for both types of solution in the gapless semiconductor are given by expressions (14) and (15), the only difference is that it is necessary to make the replacement $E - V_0 \rightarrow s\bar{u}k'$. In the above manner, let us analyze what kind of solution we have in the gapless semiconductor:

1) if $u > \bar{u}$ then at any angle $-\frac{\pi}{2} < \phi < \frac{\pi}{2}$

a) there exists the oscillating solution for electrons at $V_0 < 0$ and for holes at $V_0 > 0$ for any k ;

b) there exists the damped solution for electrons at $V_0 > 0$ and for holes at $V_0 < 0$ in

the energy intervals

$$\begin{aligned} E_0^+(\phi) < E_e < E_0^-(\phi), \\ E_0^-(\phi) < E_h < E_0^+(\phi), \end{aligned} \tag{27}$$

where $E_0^\pm(\phi) = \frac{u}{u \pm \bar{u} |\sin \phi|} V_0$; and there exists the oscillating solution beyond these intervals. If we regard V_0 as the potential barrier height [3], then we have the under-barrier oscillating solution, this fact corresponds to the Klein paradox;

2) if $u < \bar{u}$ then

a) the situation is the same as in 1) for angles $|\sin \phi| < \frac{u}{\bar{u}}$;

b) for angles $\frac{u}{\bar{u}} < |\sin \phi| < 1$, we should distinguish two particular cases:

(i) the solution is damped for electrons at $V_0 < 0$ and holes at $V_0 > 0$ for any k ;

(ii) the solution is oscillating for electrons at $V_0 > 0$ and holes at $V_0 < 0$ in energy ranges (27) but out of ones there is the damped solution.

Finally, let us consider the particular case $\Delta = 0$ and $V_0 = 0$ at $\bar{u} \neq u$:

1) if $u > \bar{u}$ then the solution is oscillating at any angle $-\frac{\pi}{2} < \phi < \frac{\pi}{2}$ and any energy, this fact corresponds to the Klein paradox;

2) if $u < \bar{u}$ then the solution is oscillating at any energy for $|\sin \phi| < \frac{u}{\bar{u}}$ and the solution is damped at $|\sin \phi| > \frac{u}{\bar{u}}$.

In conclusion, we note that the considered heterostructure can be used as the “switch”, namely, applying a voltage on the narrow-gap semiconductor ribbon we can “switch on” and “switch off” transmission of the charge carriers through range II depending on the energy range in which the Dirac point of graphene falls (in the range of the oscillating or damped solution). When we apply an electric field F , the Dirac point of graphene shifts in energy by the value $\sim eFd$ where d is a distance from the voltage applying point to the narrow-gap semiconductor ribbon. We suppose that the electric field is weak enough: $eFd < \Delta - |V_0|$, i.e. current does not flow at the given V_0 . The electric field correction results in displacement $\sim \frac{1}{2}eFD$ of extrema of the conduction and valence bands of the narrow-gap semiconductor [17]. Applying the voltage $-U_0$ to the narrow-gap semiconductor ribbon changes the difference $V'_0 = V_0 - U_0$ of work functions between the narrow-gap semiconductor and graphene so that passage of electrons becomes possible at $eFd > E^+(\phi)|_{V'_0}$. Condition of passage for holes is $eFd > |E^-(\phi)|$. Changing U_0 , we can achieve passage of either electrons or holes.

An alternative scheme of the “switch” is possible. Due to zero gap in graphene one can pump electrons from the substrate in the conduction band or displace electrons from graphene thereby obtaining holes in the valence band. Changing position of the Fermi level E_F in one of the graphene layers we can provide passage of either electrons at the condition $eFd + E_F > E^+(\phi)$ ($E_F > 0$) or holes at $-eFd + E_F < E^-(\phi)$ ($E_F < 0$).

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